R PMX Best Practices Checklist – v2

Reproducibility

- ☐ Number R scripts to reflect the order of the workflow (e.g. `Task01_ExploreData.R`, `Task02_MonolixRun.R`, `Task03_MonolixPlot.R`). Data preparation and modeling should be in separate scripts.
- ☐ When scripts depend on each other, create a parent R script (e.g. `Task00_RunAll.R`) that executes all code in order. Ensure it executes from command line using: `R-3.4.3 CMD BATCH --vanilla --slave "Task00_RunAll.R".`
- ☐ Set `echo=TRUE` when calling scripts to produce a comprehensive output file. (e.g. `source("Task01_ExploreData.R",echo=TRUE).`
- ☐ Set the random number generator seed `set.seed(123456)`
- ☐ At the top of all scripts, source an `initialize_script.R file`. This file should:
  - Declare constants upfront (never hardcode numbers). Be sure to include units and a reference, e.g. `Kd = 1.5 #nM, from Investigator's Brochure version 1, page 27.`
  - Specify in variables the paths where data is located and where results are stored. Use these variables in subsequent scripts when loading data and saving results.
  - We recommend not setting the working directory; instead just use the default working directory, which is the directory from which the code is run. If you do set the working directory, do this only once in `initialize_script.R` and ensure the `setwd()` command is general and will work for multiple users.
- ☐ At the end of all scripts, call `sessionInfo()` to document R version and all packages used.

Readability

- ☐ Follow the tidyverse style guide
  - use snake case for variables and functions (i.e. this_is_my_variable)
  - one exception to style guide: Andy prefers "=" over "<-"
- ☐ Ensure sufficient comments, especially units and references
- ☐ Create `Readme.txt` to summarize how to understand and execute your code.

Graphs

- ☐ All plots should be labeled draft unless final.
- ☐ All plots should list the program that created them and the location of graphics file output.
- ☐ Start of plot filename should match the start of the script name that created it (e.g. `Task02_ExploreData.R` would create `Task02_Spaghetti.pdf`)
- ☐ Use the tidyverse (e.g. `ggplot2`, `tidyr`, `dplyr`) so others can easily read and validate your code.
- ☐ Use a white background with faint grid lines and large, readable font. In `initialize_script.R`, these settings can be made the default with the command: `xgxr::xgx_theme_set()`

Andy Stein in collaboration with the R SME Team, Feb 13, 2018